

Ethyl heptanoate  
106-30-9 | DTXSID1040112

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.95            | 0.69 | 0.95           | 0.65 | 0.96       | 0.68 |

Model Results

Predicted value: 4.45

Global applicability domain: Inside

Local applicability domain index: 9.28e-01

Confidence level: 8.20e-01

Nearest Neighbors from the Training Set

|  |  |   |
|--|--|---|
| <div>Image not found</div> <div>Hexachloroethane</div> <div>Measured: 4.47</div> <div>Predicted: 4.45</div>    | <div>Image not found</div> <div>1,4-Dichlorobenzene</div> <div>Measured: 4.46</div> <div>Predicted: 4.45</div> | <div>Image not found</div> <div>Pentyl ether</div> <div>Measured: 4.80</div> <div>Predicted: 4.98</div> |
| <div>Image not found</div> <div>1,3-Dichlorobenzene</div> <div>Measured: 4.12</div> <div>Predicted: 4.44</div> | <div>Image not found</div> <div>1,2-Dichlorobenzene</div> <div>Measured: 4.36</div> <div>Predicted: 4.46</div> |   |